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Structure, Conductance and Strength of Atomic-Sized Iridium Wires

Tokushi Kizuka and Minoru Ryu

Institute of Materials Science, University of Tsukuba, Tsukuba 305-8573, Japan
E-mail: kizuka@ims.tsukuba.ac.jp

1. Introduction

Nanometer-sized contacts (NCs) of metals have been studied in relation to the quantized conductance that was first discovered experimentally in two dimensional electron gases at semiconductor interfaces [1]. The formation and structures of NCs showing conductances lower than a few quantum units ($G_0=2e^2/h$, where e is the charge of electron and h is Planck's constant) have been investigated by mechanically controllable break junction and nanometer-tip manipulation techniques [2]. The study of the atomic configuration, the electron transport and the mechanical properties of thinner wires, i.e., atomic-sized wires (ASWs), was conducted for gold (Au) ASWs. Most of the reports concerning the conductance of Au ASWs have proposed conductance levels of approximately 1 G_0. On the other hand, it has been reported that the conductances of some ASWs composed of other kinds of metallic element, e.g. palladium (Pd), platinum (Pt), iridium (Ir), do not necessarily correspond to this unit conductance [3]. The structures of Pd and Pt ASWs have been observed [4], although relationship between their structures and conductance was not investigated. For Ir ASWs, however, even their structure has not been observed. In this report, we studied the structure, conductance, and mechanical properties of Ir ASWs along with the relationship between structure and these properties by *in situ* high-resolution TEM.

2. Method

The experimental method used in this study was developed on the basis of *in situ* high-resolution TEM combined with subnanonewton force measurements as used in atomic force microscopy (AFM) and conductance measurements as used in scanning tunneling microscopy [5]. First, we prepared Ir tips for contact; Ir was evaporated and deposited on a nanometer-sized scanning-tip of Si cantilever. The cantilever was attached to the front of a tube piezo on a cantilever holder on a transmission electron microscope. A contact edge of an Ir plate was thinned to 5 - 20 nm by argon ion milling, and was attached to a plate holder. The cantilever and the plate holders were then inserted into the microscope. The cantilever tip was brought into contact with an edge of the opposing plate by piezo manipulation while applying a bias voltage of 39 mV between the tip and the plate. The tip was pressed into the plate to prepare NCs, and then retracted to elongate them to transform them into ASWs. The structural dynamics during the retraction was observed *in situ* by the lattice imaging by high-resolution TEM. Force applied between the tip and the plate was simultaneously measured by optical detection of cantilever deflection. The conductance was measured by a two-terminal method.

3. Results and discussion

Figure 1 shows a time sequence series of high-resolution images of the formation procedure of an Ir ASW. The cantilever-tip and the plate edge are observed in the upper and lower regions of each frame in Fig. 1, respectively. A contact boundary is observed between them in the middle of the frame. At first, the width of the contact is approximately 1 nm (Fig. 1(a)). As the cantilever-tip was retracted from the plate, the width decreases by slip (Figs. 1(a) - 1(c)), and finally reaches to a single-atom width (Fig. 1(d)). This wire is composed of three atoms with an interatomic distance of 0.23 $\pm$ 0.05 nm. The shape is straight along the retraction direction of the cantilever-tip.

Figure 2 shows the variations in parameters during the procedure observed in Fig. 1 as a function of time. The parameters are the strain and the minimum cross-sectional area of the wire, the force and the stress applied to the wire, and the current and the current density through the wire. The times associated with triangles a - d in Fig. 2 (hereafter time a, b, c and d) correspond to the times at which each image in Figs. 1(a) - 1(d) were observed. The strain was estimated from the variation in distance between the cantilever-tip and the plate. We assumed that the shape of the cross section of the wire at a minimum width is circular, and measured this

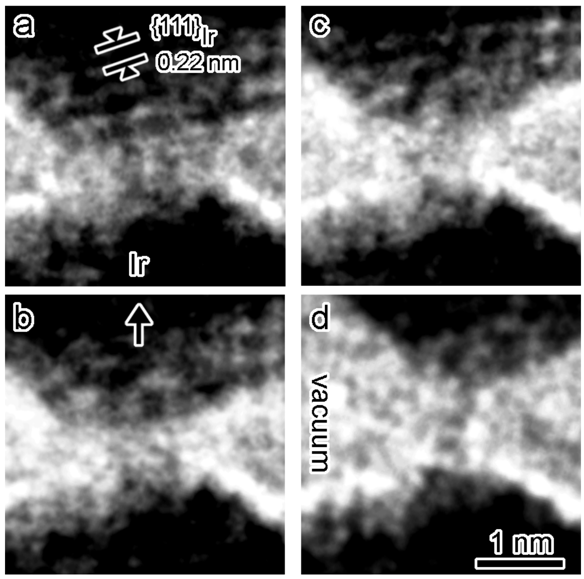

Fig. 1 Time-sequence series of high-resolution images of elongation of Ir nanometer-sized contact (a-c) and successive growth of wire of single atom width (d).

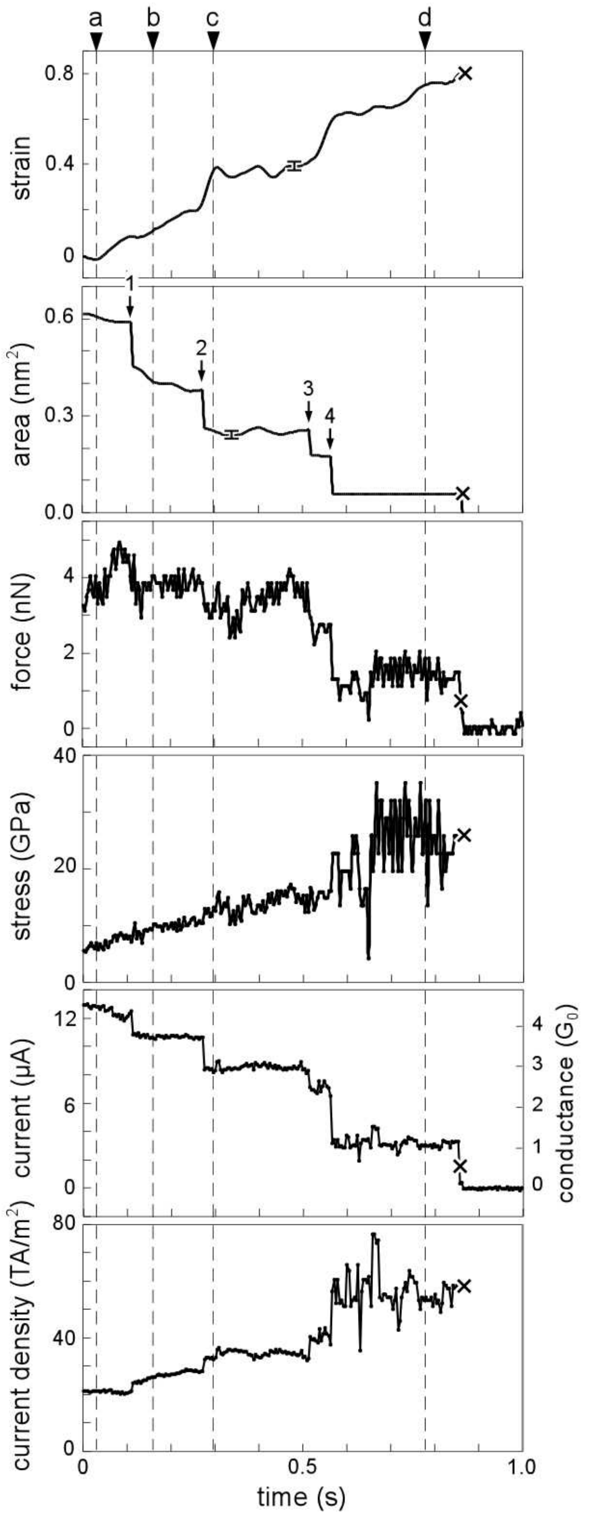

Fig. 2 Variations in strain, force, minimum cross-sectional area, force, current (with conductance) and current density during tensile deformation observed in Fig. 1 as a function of time. Arrows with numbers represent the times that slip occurred. Crosses (x) indicate fracture.

width from the images. We calculated the stress by dividing the force by the minimum cross-sectional area. Slip was observed, and the times at slip are indicated by arrows in the uppermost frame of Fig. 2.

In Fig. 2, the variation in current resembles that of the minimum cross-sectional area, showing the current is dominated by the constriction. The current density ranges from 20 to 60 TA/m^2.

The tensile strength of the ASW, i.e. the maximum stress observed, is 35 $\pm$ 17 GPa, as shown in Fig. 2. To develop analyses based on the mechanics of materials for this wire, we derived the stress-strain relation for the tensile deformation observed in Fig. 1. The Young's modulus of the Ir NC was 20 $\pm$ 11 GPa, whereas the modulus of the ASW was 90 $\pm$ 55 GPa. Thus, the Young's modulus of the Ir ASW was 4.5 times larger than that of the Ir NC.

4. Conclusion

We have performed the experiment on the mechanics of materials on an atomic scale for Ir ASWs by *in situ* TEM. From the measurement of stress-strain relations, the change in the mechanical properties owing to the size reduction to nanometer-scale and atomistic-scale were elucidated.

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